

Access DB# 29241

# SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: TRUONG, Duc Examiner #: 69352 Date: 8/6/04  
Art Unit: 1211 Phone Number 302-1681 Serial Number: 10678782  
Mail Box and Bldg/Room Location: 10271 Results Format Preferred (circle) PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

\*\*\*\*\*  
Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: \_\_\_\_\_

Inventors (please provide full names): \_\_\_\_\_

Earliest Priority Filing Date: \_\_\_\_\_

*\*For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional, or issue) appropriate serial number.*

Formula of claim 1. - Sharks

RELATED TO  
REQUEST  
#129279

SCIENTIFIC REFERENCE BR  
Sci. & Tech. Info. Cntr

AUG 6

Pat. & T.M. Office

## STAFF USE ONLY

Searcher: EL  
Searcher Phone #: \_\_\_\_\_  
Searcher Location: \_\_\_\_\_  
Date Searcher Picked Up: \_\_\_\_\_  
Date Completed: 8-13-04  
Searcher Prep & Review Time: \_\_\_\_\_  
Clerical Prep Time: \_\_\_\_\_  
Online Time: \_\_\_\_\_

### Type of Search

NA Sequence (#) \_\_\_\_\_  
AA Sequence (#) \_\_\_\_\_  
Structure (#) \_\_\_\_\_  
Bibliographic \_\_\_\_\_  
Litigation \_\_\_\_\_  
Fulltext \_\_\_\_\_  
Patent Family \_\_\_\_\_  
Other \_\_\_\_\_

### Vendors and cost where applicable

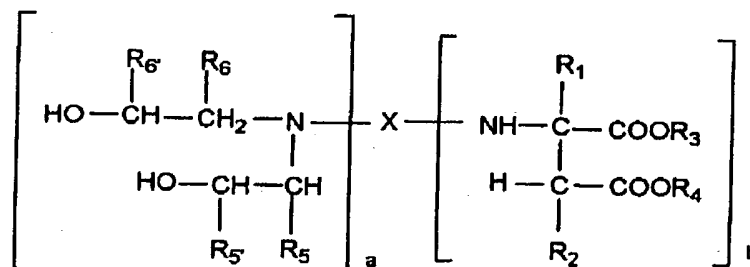
STN \_\_\_\_\_  
Dialog \_\_\_\_\_  
Questel/Orbit \_\_\_\_\_  
Dr.Link \_\_\_\_\_  
Lexis/Nexis \_\_\_\_\_  
Sequence Systems \_\_\_\_\_  
WWW/Internet \_\_\_\_\_  
Other (specify) \_\_\_\_\_

PO7926

-15-

WHAT IS CLAIMED IS:

1. An aspartate of the formula:



where

5

X represents an m-valent organic residue obtained by removing the primary amino group or groups from a mono or polyamine which has (cyclo)aliphatically bound amino groups and a number average molecular weight of 60 to 6000, and which may contain further functional groups that either are reactive with isocyanate groups or are inert to isocyanate groups at temperatures of up to 100°C,

10

R<sub>1</sub> and R<sub>2</sub> may be identical or different and represent hydrogen or organic groups which are inert towards isocyanate groups at a temperature of 100°C or less,

15

R<sub>3</sub> and R<sub>4</sub> may be identical or different and represent organic groups which are inert towards isocyanate groups at a temperature of 100°C or less,

20

R<sub>5</sub> represents hydrogen or together with R<sub>5</sub> and the carbon atoms to which they are connected forms a six-membered cycloalkyl group, with said cycloalkyl group being substituted with from 0 to 3 alkyl groups having from 1 to 3 carbon atoms,

25

PO7926

-16-

5

$R_5$  represents a moiety selected from the group consisting of  
i)  $C_1$  to  $C_8$  alkyl groups which may be interrupted with an  
oxygen atom, ii)  $C_6$  to  $C_{10}$  aryl groups, which may be  
substituted with up to three alkyl groups having from 1 to 3  
carbon atoms and iii)  $C_6$  to  $C_{12}$  cycloalkyl groups, which may  
be substituted with up to three alkyl groups having from 1 to  
3 carbon atoms,

10

$R_6$  represents hydrogen or together with  $R_5$  and the carbon  
atoms to which they are connected forms a six-membered  
cycloalkyl group, with said cycloalkyl group being substituted  
with from 0 to 3 alkyl groups having from 1 to 3 carbon  
atoms,

15

$R_6$  represents a moiety selected from the group consisting of  
i)  $C_1$  to  $C_8$  alkyl groups which may be interrupted with an  
oxygen atom, ii)  $C_6$  to  $C_{10}$  aryl groups, which may be  
substituted with up to three alkyl groups having from 1 to 3  
carbon atoms and iii)  $C_6$  to  $C_{12}$  cycloalkyl groups, which may  
be substituted with up to three alkyl groups having from 1 to  
3 carbon atoms,

20

with the proviso that  $R_5$  and  $R_6$  are the same and  $R_5$  and  $R_6$  are the  
same, and

25

a and b represent integers of from 1 to 5, provided that the sum of a  
and b is from 2 to 6.

=> file reg

FILE 'REGISTRY' ENTERED AT 12:00:12 ON 13 AUG 2004  
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FILE 'REGISTRY' ENTERED AT 11:44:35 ON 13 AUG 2004  
 ACT TRU782/A

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 L1 STR  
 L2 1 SEA FILE=REGISTRY SSS SAM L1  
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 L3 33 S L1 FUL  
 SAV L3 TRU782/A

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 L4 STR L1

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 L5 1 S L4 SSS SAM SUB=L3  
 L6 20 S L4 SSS FUL SUB=L3  
 SAV L6 TRU491/A  
 L7 13 S L3 NOT L6

FILE 'CAOLD' ENTERED AT 11:56:22 ON 13 AUG 2004  
 L8 0 S L6

FILE 'ZCAPLUS' ENTERED AT 11:56:28 ON 13 AUG 2004  
 L9 10 S L6

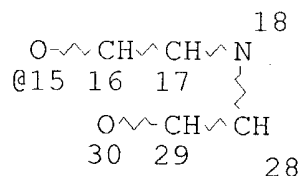
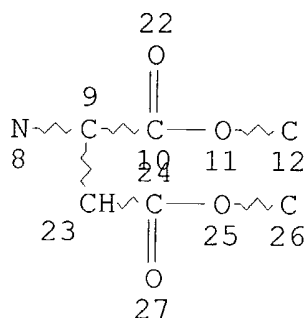
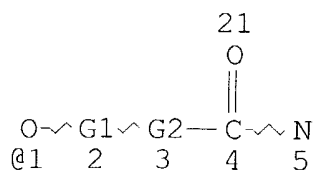
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FILE 'ZCAPLUS' ENTERED AT 11:56:58 ON 13 AUG 2004  
 L11 7 S L7

FILE 'REGISTRY' ENTERED AT 12:00:12 ON 13 AUG 2004

=> d l3 que stat

L1 STR



G3 20

REP G1=(2-5) C  
 REP G2=(0-1) O  
 VAR G3=15/1  
 NODE ATTRIBUTES:  
 NSPEC IS RC AT 12  
 NSPEC IS RC AT 26  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE  
 L3 33 SEA FILE=REGISTRY SSS FUL L1

100.0% PROCESSED 22270 ITERATIONS  
 SEARCH TIME: 00.00.01

33 ANSWERS

=> file zcaplus  
 FILE 'ZCAPLUS' ENTERED AT 12:00:25 ON 13 AUG 2004  
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

=> d l11 1-7 cbib abs hitstr hitrn

L11 ANSWER 1 OF 7 ZCAPLUS COPYRIGHT 2004 ACS on STN

1996:189805 Document No. 124:306014 Kinetic studies and analytical determinations on some derivatives of L-asparagic acid acting as antimetabolites and alkylating agents. Sunel, Valeriu; Cecal, Alexandru; Soldea, Camelia; Asandei, Nicolae (Fac. Chem., "Al. I. Cuza" Univ., Iasi, 6600, Rom.). Revue Roumaine de Chimie, 40(7-8), 773-8 (English) 1995. CODEN: RRCHAX. ISSN: 0035-3930. Publisher: Editura Academiei Romane.

AB The kinetics of reactions between silver nitrate (110AgNO3) and some antimetabolites and alkylating agents supported by  $\alpha,\beta$ -diesters of N-(p-aminobenzoyl)-L-asparagic acid was studied. An anal. method is advanced for detg. the concn. of these org. compds. by titrn. with 110AgNO3 soln. of a known concn.

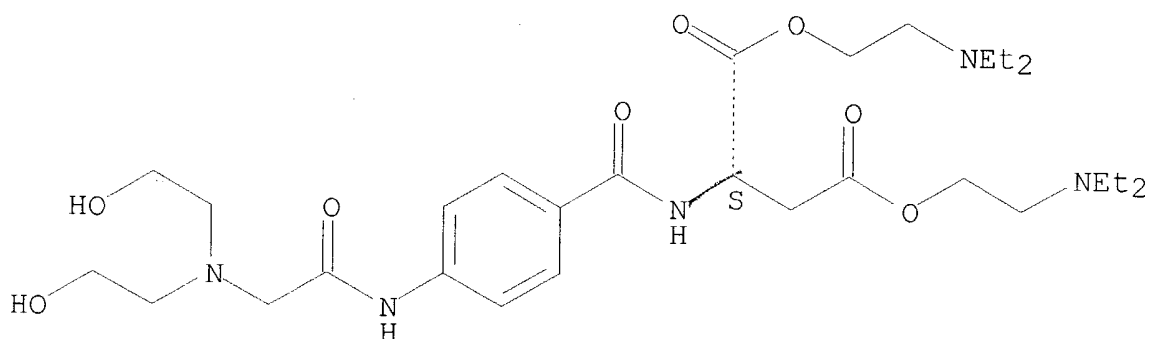
IT 144075-66-1 144075-67-2 176174-93-9  
176174-94-0

(kinetic studies and anal. detns. on some derivs. of L-asparagic acid acting as antimetabolites and alkylating agents)

RN 144075-66-1 ZCAPLUS

CN L-Aspartic acid, N-[4-[[[bis(2-hydroxyethyl)amino]acetyl]amino]benzoyl]-, bis[2-(diethylamino)ethyl] ester (9CI) (CA INDEX NAME)

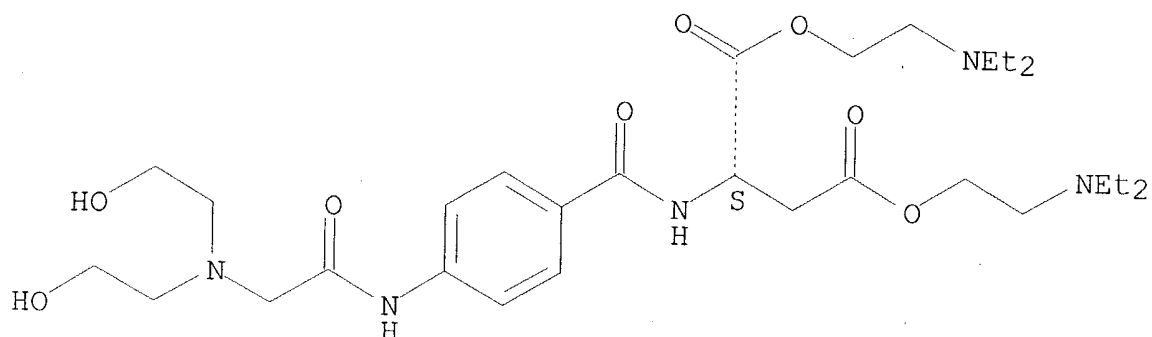
Absolute stereochemistry.



RN 144075-67-2 ZCAPLUS

CN L-Aspartic acid, N-[4-[[[bis(2-hydroxyethyl)amino]acetyl]amino]benzoyl]-, bis[2-(diethylamino)ethyl] ester, monohydrochloride (9CI) (CA INDEX NAME)

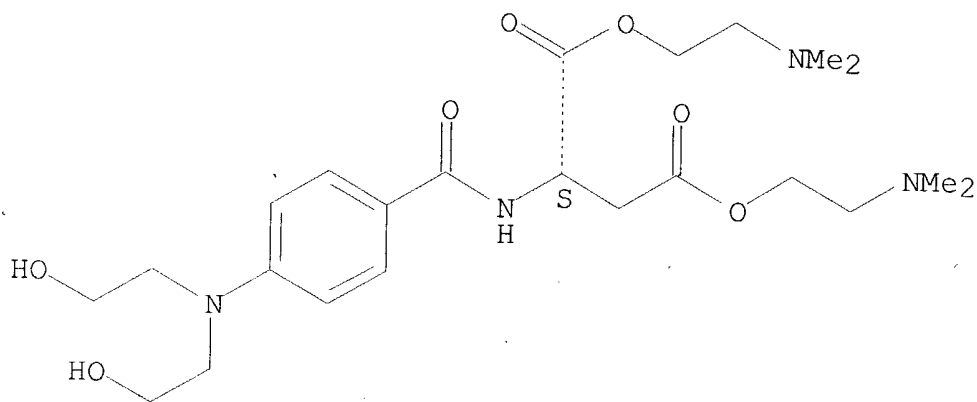
Absolute stereochemistry.



● HCl

RN 176174-93-9 ZCAPLUS  
 CN L-Aspartic acid, N-[4-[bis(2-hydroxyethyl)amino]benzoyl]-, bis[2-(dimethylamino)ethyl] ester, monohydrochloride (9CI) (CA INDEX NAME)

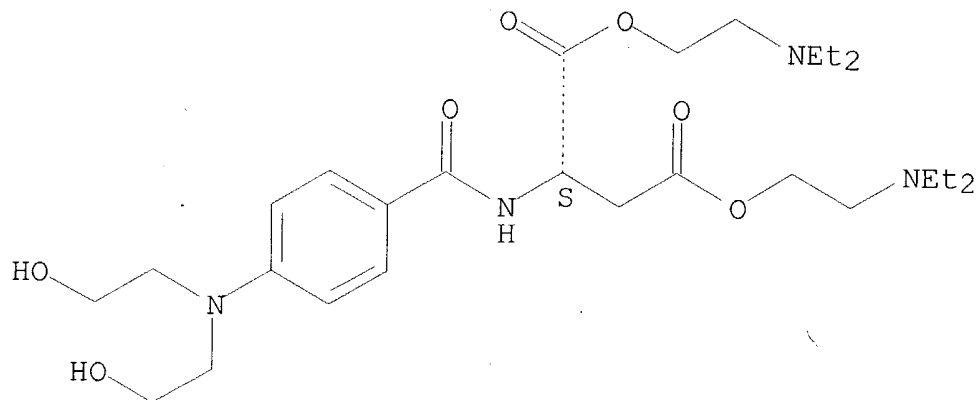
Absolute stereochemistry.



● HCl

RN 176174-94-0 ZCAPLUS  
 CN L-Aspartic acid, N-[4-[bis(2-hydroxyethyl)amino]benzoyl]-, bis[2-(diethylamino)ethyl] ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



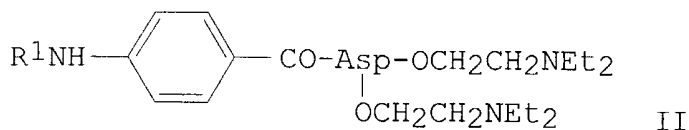
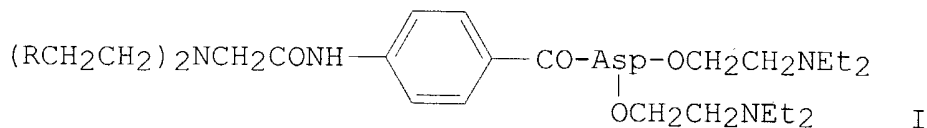
● HCl

IT 144075-66-1 144075-67-2 176174-93-9  
176174-94-0

(kinetic studies and anal. detns. on some derivs. of L-asparagic acid acting as antimetabolites and alkylating agents)

L11 ANSWER 2 OF 7 ZCAPLUS COPYRIGHT 2004 ACS on STN  
1992:612928 Document No. 117:212928 Synthesis of anticancerous substances. Sunel, Valeriu; Cecal, A. (Dep. Macromol. Org. Chem., Polytech. Inst., Iasi, Rom.). Buletinul Institutului Politehnic din Iasi, Sectia 2: Chimie si Inginerie Chimica, 36(3-4), 57-62 (English) 1990. CODEN: BPICDV. ISSN: 0254-7104. OTHER SOURCES: CASREACT 117:212928.

GI





AB N-mustard tripeptide I.HCl (R = Cl) was prepd. from aspartate II (R1 = H) in 4 steps. Thus, II (R1 = H) was acylated with ClCH<sub>2</sub>COC1 in benzene contg. pyridine to give 78.2% II (R1 = ClCH<sub>2</sub>CO), which was treated with diethanolamine in the presence of KI and AcONa in acetone to give 70.7% I (R = OH). The latter was treated with HCl in EtOH to give 72.3% I.HCl (R = OH), which was chlorinated with PCl<sub>5</sub> in CHCl<sub>3</sub> to give 58.8% I.HCl (R = Cl).

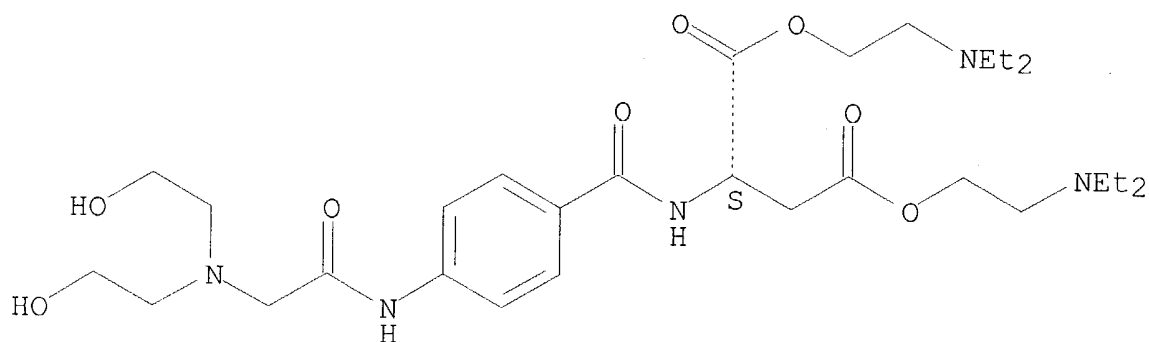
IT 144075-67-2P

(prepn. and chlorination of)

RN 144075-67-2 ZCAPLUS

CN L-Aspartic acid, N-[4-[[[bis(2-hydroxyethyl)amino]acetyl]amino]benzoyl]-, bis[2-(diethylamino)ethyl] ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

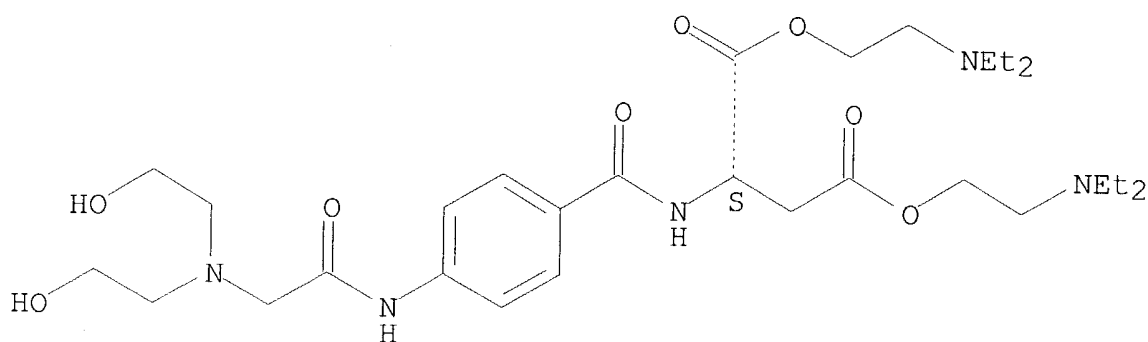
IT 144075-66-1P

(prepn. and conversion of, to monohydrochloride)

RN 144075-66-1 ZCAPLUS

CN L-Aspartic acid, N-[4-[[[bis(2-hydroxyethyl)amino]acetyl]amino]benzoyl]-, bis[2-(diethylamino)ethyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 144075-67-2P

(prepn. and chlorination of)

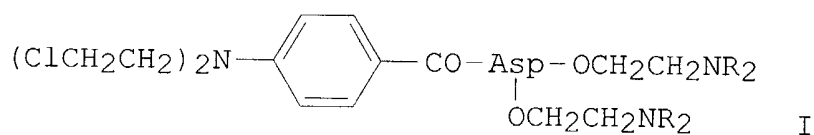
IT 144075-66-1P

(prepn. and conversion of, to monohydrochloride)

L11 ANSWER 3 OF 7 ZCAPLUS COPYRIGHT 2004 ACS on STN

1987:598866 Document No. 107:198866 Synthesis of some nitrogen yperites as N-(p-aminobenzoyl)-L-aspartic acid esters. Sunel, Valeriu; Ciugureanu, Constantin; Budeanu, Constantin (Fac. Tehnol. Chim., Inst. Politeh., Iasi, Rom.). Revistade Chimie (Bucharest, Romania), 37(10), 855-9 (Romanian) 1986. CODEN: RCBUAU. ISSN: 0034-7752.

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AB Nitrogen yperite-type compds. I (R = Me, Et) were prepd. from aspartic acid by sequential acylation with p-O2NC6H4COCl, esterification with HOCH2CH2NR2, catalytic hydrogenation of the nitro group, hydroxyethylation with ethylene oxide, and chlorination with POCl3.

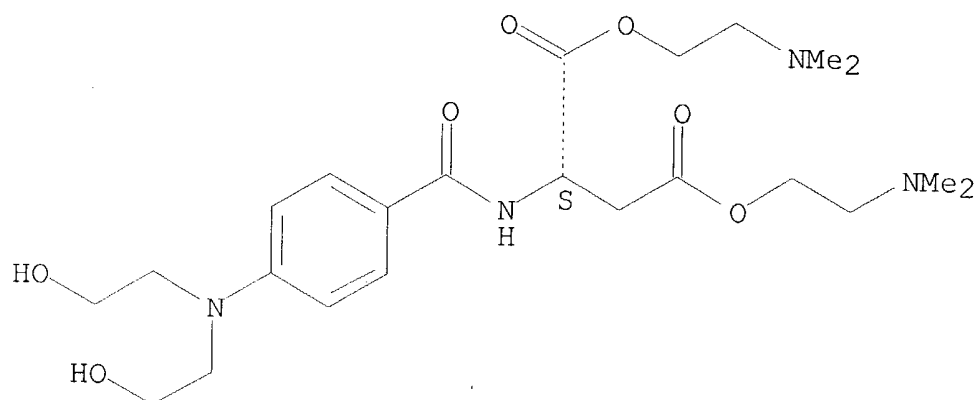
IT 110976-60-8P 110976-61-9P

(prepn. and chlorination-dehydroxylation of)

RN 110976-60-8 ZCAPLUS

CN L-Aspartic acid, N-[4-[bis(2-hydroxyethyl)amino]benzoyl]-, bis[2-(dimethylamino)ethyl] ester (9CI) (CA INDEX NAME)

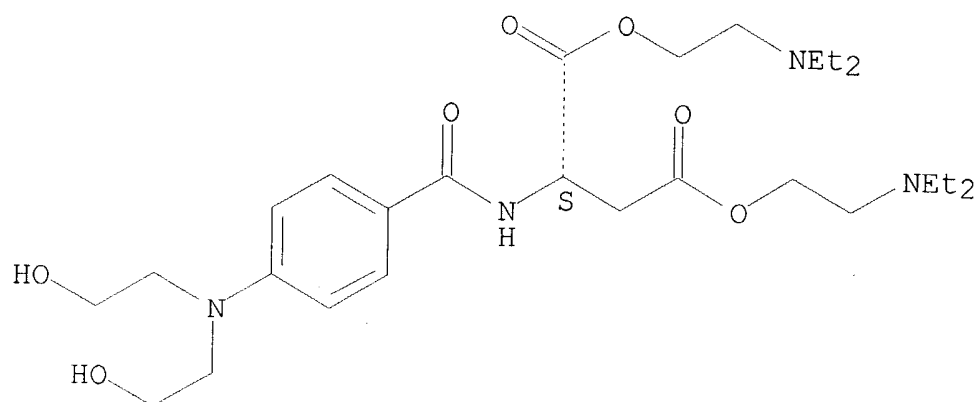
Absolute stereochemistry.



RN 110976-61-9 ZCAPLUS

CN L-Aspartic acid, N-[4-[bis(2-hydroxyethyl)amino]benzoyl]-, bis[2-(diethylamino)ethyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 110976-60-8P 110976-61-9P  
(prepn. and chlorination-dehydroxylation of)

L11 ANSWER 4 OF 7 ZCAPLUS COPYRIGHT 2004 ACS on STN  
1983:540378 Document No. 99:140378 Synthesis of antitumor compounds.  
Synthesis of diethyl N-[p-[[bis(β-chloroethyl)glycyl]amino]benzoyl]-L-aspartate hydrochloride. Sunel, Valeriu; Cecal, Alexandru (Fac. Tehnol. Chim., Inst. Politeh. Iasi, Iasi, Rom.). Revistade Chimie (Bucharest, Romania), 34(5), 394-7 (Romanian) 1983. CODEN: RCBUAU. ISSN: 0034-7752.

AB The title N-mustard (I) was prepd. from di-Et N-(p-aminobenzoyl)-L-aspartate by sequential chloroacetylation, bis(hydroxyethyl)amination, and chlorination. The bis(β-chloroethyl)amine group should confer a low toxicity and

high antitumor activity (no data) to the tripeptide residue. I and intermediates in its prepn. were characterized by their IR and UV spectra.

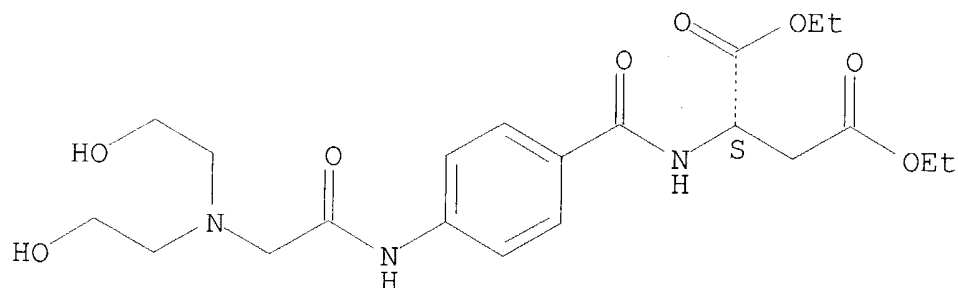
IT 86590-49-0P

(prepn. and chlorination of)

RN 86590-49-0 ZCAPLUS

CN L-Aspartic acid, N-[4-[[[bis(2-hydroxyethyl)amino]acetyl]amino]benzoyl]-, diethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

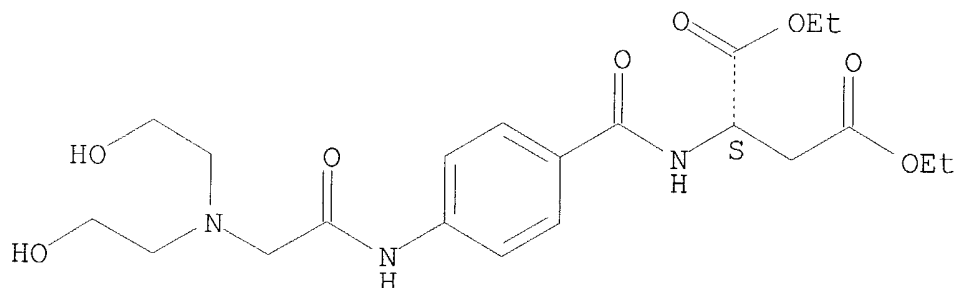
IT 86590-50-3P

(prepn. of)

RN 86590-50-3 ZCAPLUS

CN L-Aspartic acid, N-[4-[[[bis(2-hydroxyethyl)amino]acetyl]amino]benzoyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 86590-49-0P

(prepn. and chlorination of)

IT 86590-50-3P

(prepn. of)

L11 ANSWER 5 OF 7 ZCAPLUS COPYRIGHT 2004 ACS on STN

1983:459532 Document No. 99:59532 Kinetic and analytical study on precipitation reactions with silver-110 nitrate of some di-( $\beta$ -chloroethyl)amine derivates and hydrochlorides with esters of N-(p-aminobenzoyl)-L-aspartic acid as carriers from dimethylformamide-water solution. Cecal, A.; Sunel, V.; Ghimiciu, L. (Fac. Chem. Technol., Polytech. Inst. Iasi, Iasi, 6600, Rom.). Journal of Radioanalytical Chemistry, 78(2), 247-53 (English) 1983. CODEN: JRACBN. ISSN: 0022-4081.

AB The kinetics of pptn. reactions with  $^{110}\text{AgNO}_3$  of some di( $\beta$ -chloroethyl)amine derivs. and hydrochlorides with esters of N-(p-aminobenzoyl)-L-aspartic acid as carriers in aq. DMF were studied. The rate consts. of these reactions are of the order of  $10^{-4} \text{ M}^{-1}\text{min}^{-1}$ . The concns. of the corresponding hydrochloride solns. were measured by radiometric titrn. with  $^{110}\text{AgNO}_3$  soln. of known concn.

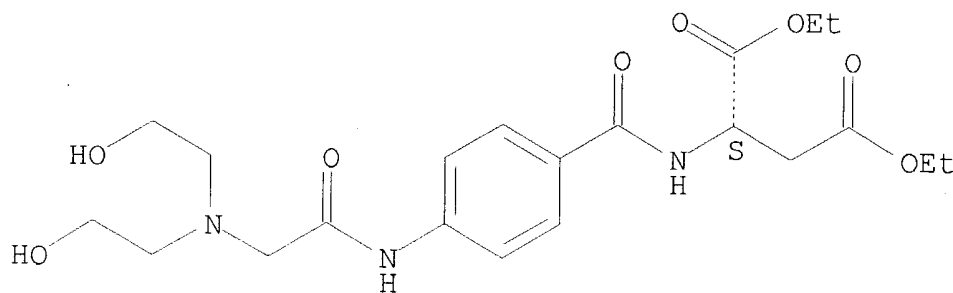
IT 86590-49-0 86590-50-3

(reaction of, with silver nitrate, pptn. kinetics in)

RN 86590-49-0 ZCAPLUS

CN L-Aspartic acid, N-[4-[[[bis(2-hydroxyethyl)amino]acetyl]amino]benzoyl]-, diethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

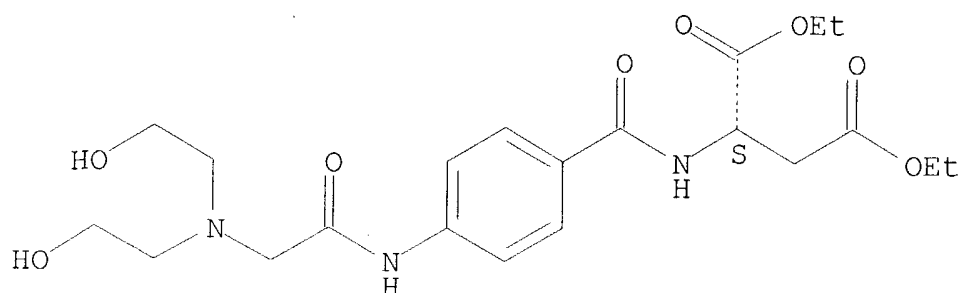


● HCl

RN 86590-50-3 ZCAPLUS

CN L-Aspartic acid, N-[4-[[[bis(2-hydroxyethyl)amino]acetyl]amino]benzoyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 86590-49-0 86590-50-3

(reaction of, with silver nitrate, pptn. kinetics in)

L11 ANSWER 6 OF 7 ZCAPLUS COPYRIGHT 2004 ACS on STN

1983:198688 Document No. 98:198688 New derivatives of

N-(p-aminobenzoyl)-L-aspartic acid with potential antitumor effect. Sunel, Valeriu; Apostolescu, Maria; Budeanu, Constantin; Danet, Dumitru (Inst. Politeh., Iasi, Rom.). Revistade Chimie (Bucharest, Romania), 33(12), 1099-101 (Romanian) 1982. CODEN: RCBUAU. ISSN: 0034-7752.

AB p-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CO-Asp-OH was esterified to give p-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CO-Asp(OR)-OR (R = Bu, EtCHMe, Pr, Me<sub>2</sub>CH), which were hydroxyethylated with ethylene oxide to give the corresponding p-(HOCH<sub>2</sub>CH<sub>2</sub>)<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CO-Asp(OR)-OR.

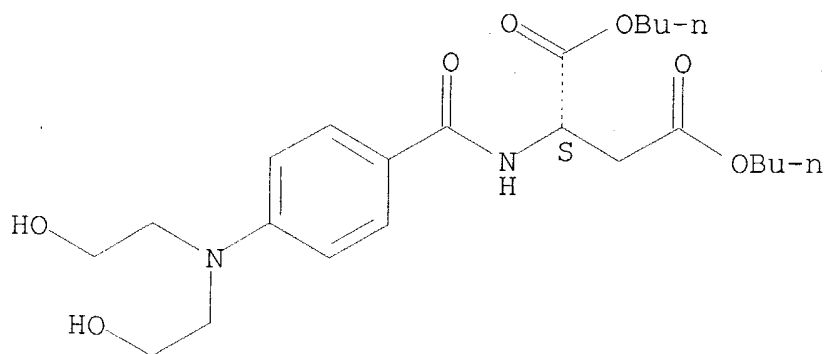
IT 85574-53-4P 85574-54-5P 85574-55-6P  
85574-56-7P

(prepn. of)

RN 85574-53-4 ZCAPLUS

CN L-Aspartic acid, N-[4-[bis(2-hydroxyethyl)amino]benzoyl]-, dibutyl ester (9CI) (CA INDEX NAME)

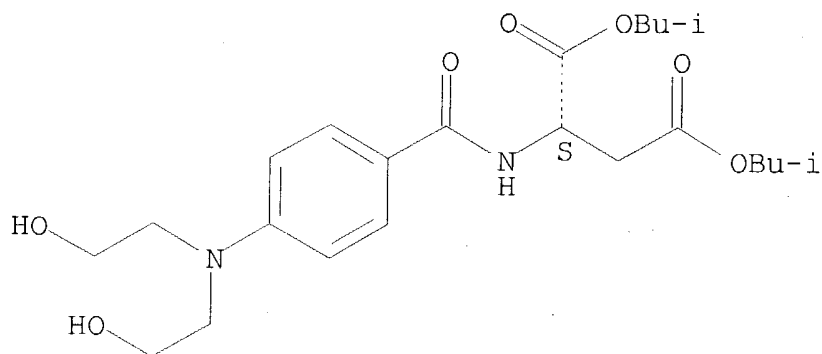
Absolute stereochemistry.



RN 85574-54-5 ZCAPLUS

CN L-Aspartic acid, N-[4-[bis(2-hydroxyethyl)amino]benzoyl]-, bis(2-methylpropyl) ester (9CI) (CA INDEX NAME)

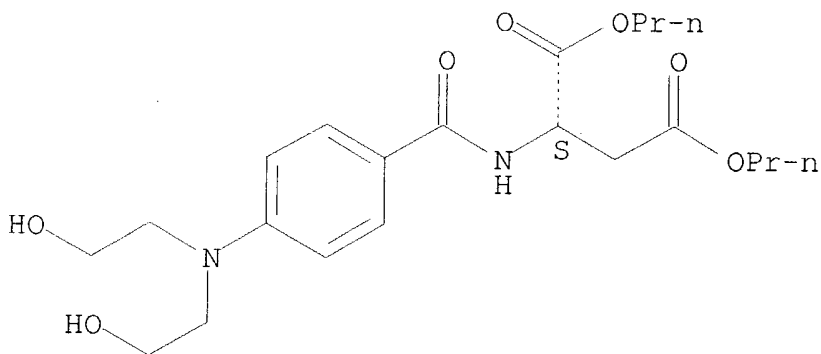
Absolute stereochemistry.



RN 85574-55-6 ZCAPLUS

CN L-Aspartic acid, N-[4-[bis(2-hydroxyethyl)amino]benzoyl]-, dipropyl ester (9CI) (CA INDEX NAME)

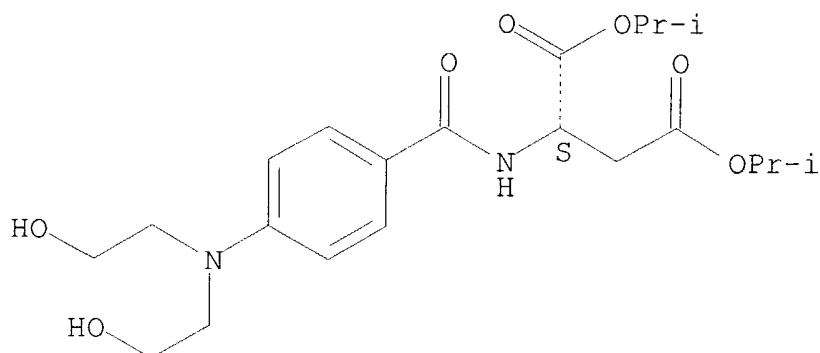
Absolute stereochemistry.



RN 85574-56-7 ZCAPLUS

CN L-Aspartic acid, N-[4-[bis(2-hydroxyethyl)amino]benzoyl]-, bis(1-methylethyl) ester (9CI) (CA INDEX NAME)

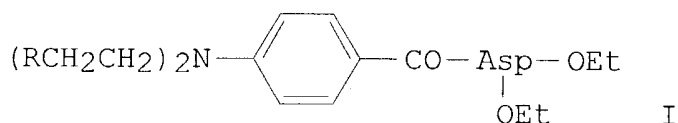
Absolute stereochemistry.



IT 85574-53-4P 85574-54-5P 85574-55-6P  
85574-56-7P  
(prepn. of)

L11 ANSWER 7 OF 7 ZCAPLUS COPYRIGHT 2004 ACS on STN  
1980:198735 Document No. 92:198735 Syntheses of anticancer substances.  
XXI. Synthesis of the diethyl ester of p-[di( $\beta$ -chloroethyl)amino]benzoyl-L-aspartic acid with potential anticancer action. Sunel, Valeriu; Budeanu, C. H.; Mazilu, I.; Apostolescu, Maria (Dep. Macromol. Org. Chem., Polytech. Inst., Iasi, Rom.). Buletinul Institutului Politehnic din Iasi, Sectia 2: Chimie si Inginerie Chimica, 25(1-2), 85-9 (English) 1979. CODEN: BPICDV. ISSN: 0254-7104.

GI



I

AB The title compd. (I, R = Cl) (II) was prepd. by esterifying p-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CO-Asp-OH with EtOH, treating the resulting di-Et ester with ethylene oxide, and chlorinating the resulting I (R = OH) with SOCl<sub>2</sub>. II caused regression of Guerin tumor.

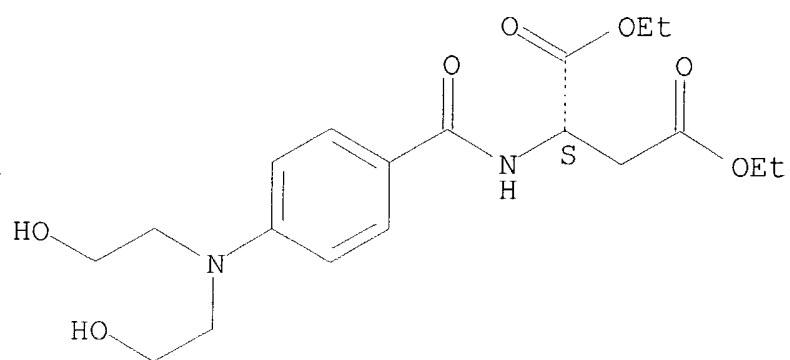
IT 73535-47-4P  
(prepn. and chlorination of)

RN 73535-47-4 ZCAPLUS

CN L-Aspartic acid, N-[4-[bis(2-hydroxyethyl)amino]benzoyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.





IT 73535-47-4P  
(prepn. and chlorination of)